# Cesium-induced Ethanol Synthesis by $CO_2$ Hydrogenation on Cu/ZnO($000\bar{1}$) Surface

## Scientific Achievement

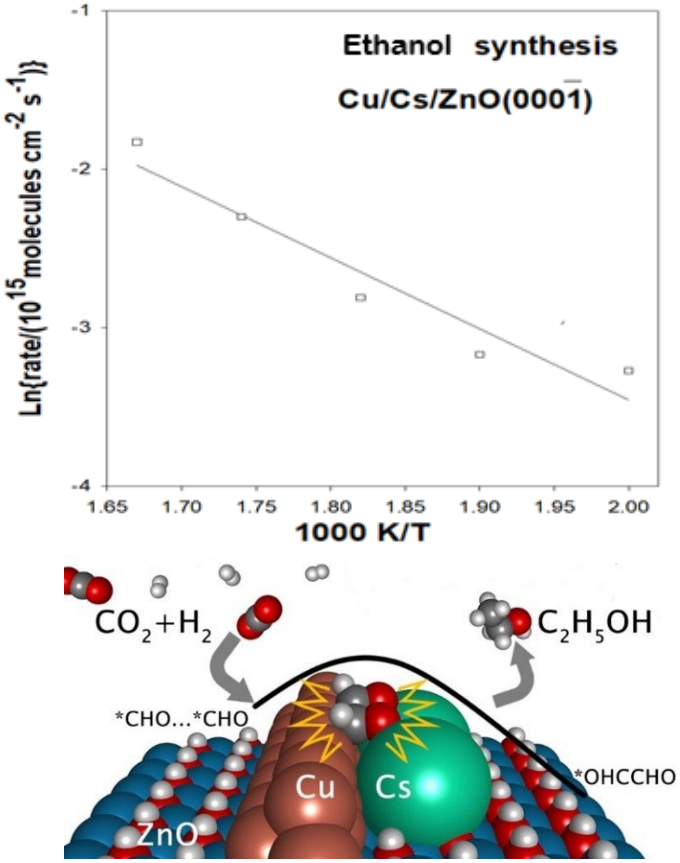
**Researchers demonstrated that Cs doping on a Cu/Zn($000\bar{1}$) surface, a model $CO_2$ conversion catalyst, opened a direct catalytic pathway to ethanol synthesis by tuning selective binding of key intermediates to enable C-C coupling and to improve methanol synthesis.**

## Significance and Impact

**Conversion of greenhouse gas $CO_2$ into higher alcohols is desirable for sustainable fuels. The Cu/ZnO/$Al_2O_3$ catalyst is the dominant industrial catalyst for methanol synthesis by $CO_2$ hydrogenation. This work shows Cs doping of the catalyst has promise for higher alcohols and gives a mechanistic basis for further improvements.**

## Research Details

- **Catalytic testing confirmed ethanol synthesis activity.**
- **X-ray photoemission spectroscopy (XPS) identified a change in the reaction mechanism for $CO_2$ to oxygenates by Cs deposition on Cu/ZnO($000\bar{1}$).**
- **Density functional theory (DFT) and kinetic Monte Carlo (KMC) simulation showed Cs-tuned binding of *CHO to facilitate further hydrogenation to methanol and open a new route toward ethanol synthesis via *OHC-CHO coupling.**




**Top:** Arrhenius plot for ethanol synthesis from $CO_2$ and $H_2$ at 0.5 atm of $CO_2$ and 4.5 atm of $H_2$; **Bottom:** Structures of Cu-Cs-ZnO interface on Cu/Cs/ZnO($000\bar{1}$) surface, active for C-C coupling and ethanol synthesis.

X. Wang, P. J. Ramírez, W. Liao, J. A. Rodriguez, and P. Liu, *JACS.* 143, 13103 (2021) (Front cover) .

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